CBPF-NF-048/95

Green Functions for Spin Clusters via Computer Algebra

R.R. Sobral[†] *and X. A. da Silva*
Centro Brasileiro de Pesquisas Físicas - CBPF
Rua Dr. Xavier Sigaud, 150
22.290-180 Rio de Janeiro/RJ, Brasil

Abstract

Green Functions for spin clusters (from two to five spins, with quantum numbers $S = 1/2$ and $S = 1$) were analytically derived and excitation energies (the poles of the Green Functions) directly revealed. An extended representation of the spin operators made it possible to deal with the Green functions equations of motion algebraically, allowing the use of simple computer algebra techniques to deduce the exact Green Functions; computer algebra also proved to be effective in obtaining energy levels and statistical average values. The values of the energies of the levels and the transition energies increase with the size of the cluster; clusters of equal number of spins but with different geometries have the same transition energies, however, the more symmetrical ones have energy degeneracies.

Key-words: Green function; Magnetism; Cluster of spins.

[†]Present address: Laboratoire Louis Néel, Centre National de la Recherche Scientifique, Boîte Postale 166, 38042 Grenoble CEDEX 9, France. CNPq post-doctoral fellowship.

1. Introduction

The double-time temperature-dependent Green Functions (GF) and their equations of motion were very popular in the sixties and seventies as a useful tool in the handling of many-body effects, particularly in the evaluation of statistical quantities of interest to Magnetism, either localized[1,2] or itinerant[3,4] from model hamiltonians with translational symmetry. A recent review is given by Irkhin[5] et al..Apart from the two-spin problem(two spins coupled by an exchange interaction) the GF method has not been applied to finite systems, although the study of cluster of spins under the action of effective magnetic fields is a well known approach to the magnetism of solids(see e.g. Smart[6]).

The two spin system was investigated using the GF technique primarily for teaching purposes:Patterson[7] et al. critically examined the handicaps of the decoupling approximation and Lucas[8] showed how to derive an exact equation(for $S = 1/2$); Ramos[9] et al. employed the two-spin system to discuss the advantage of using anticommutators GF.One may wonder why only $S = 1/2$; why not larger spin clusters?

In this paper we want to revisit the use of the method of the GF applied to clusters of spin ($S = 1/2$ and $S = 1$) introducing an extended representation for the spins operators which allows the computation of comutators with the help of simple Computer Algebra (CA). We will consider several cases: from the two-spin problem ($S = 1/2$ and $S = 1$) to the three, four and five spin clusters. We concentrate in obtaining the analytical excitation energies, which are derived from the GF for each cluster; also the energy levels and statistical mean values will be discussed.

The paper goes like this:in the next section we briefly sketch the essence of the method of the GF and its equation of motion, and introduce the extended representation of the spin operators, which will enable us to compute the commutators of these operators with the model Hamiltonian, using CA. In section 3, exact results for the GF and the excitation energies thereof derived for several spin clusters are listed. In section four, CA is used to obtain the energy spectra for some of the clusters and also the statistical mean values which occur in the GF of the three spin cluster are considered. Finally, in section five, we summarize the results.

2. Green Function for the Two-Spin System ($S = 1/2$ and $S = 1$)

We consider a set of spins (each spins identified by a site label i) interacting via a Heisenberg Hamiltonian

$$\mathcal{H} \ = \ -2J\sum_{i,j}\mathbf{S}_i.\mathbf{S}_j - \mu h\sum_{i}^{n}\mathbf{S}_i^z \tag{1}$$

where J is the exchange parameter, h an applied magnetic field, μ the Bohr magneton and $\mathbf{S}_i$ the spin operator associated to the site i, with components S_i^+, S_i^- and S_i^z. The double-time temperature dependent GF, discussed by Zubarev[1]0 and here represented by $\langle S_i^+ \mid S_j^-\rangle$, obeys the equation

$$w\langle S_i^+ \mid S_j^-\rangle \ = \ \frac{1}{2\pi}\langle[S_i^+, S_j^-]_-\rangle + \langle[S_i^+, \mathcal{H}]_- \mid S_j^-\rangle \qquad . \tag{2}$$

The problem with equation (2) is that the second term in the right hand side is a new GF for which equation 2 also applies; as a result we will have a set of chained equations. If one succeeds in solving for $\langle S_i^+ \mid S_j^-\rangle$, one may obtain, from its poles, the excitation energies; also the statistical average $\langle S_j^- S_i^+\rangle$[1]0.

For the two-spin case (with $S = 1/2$), these equations were explicitly written by Lucas[8] and an exact expression for $\langle S_1^+ \mid S_1^-\rangle$ was derived. From the details of Lucas' paper we immediately figure out that a major algebraic difficulty in applying the GF method to clusters of spins (other than the two-spin case and for other values of S than 1/2) is the computation, by standard techniques, of $[S_i^+, \mathcal{H}]_-$, $[[S_i^+, \mathcal{H}]_-, \mathcal{H}]_-$, etc, and the rearranging of the appropriate GF, generated in the process.

The following proposal allows the solution to this problem in a systematic way for more complex clusters than the two-spin ($S = 1/2$) system. For convenience, in this section, we focus on the two-spin ($S = 1/2$) paradigm. The method is easily extended to other clusters (see section 3).

Let us define the extended spins operators: S_i^+, S_i^- and S_i^z ($i = 1, 2$)

$$S_1^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \ = \ \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{3}$$

$$S_2^+ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4}$$

and similar expressions for S_i^-, and S_i^z $(i = 1, 2)$, the direct product expansion symbol $\otimes$ being defined as

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \otimes \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} Aa & Ab & Ba & Bb \\ Ac & Ad & Bc & Bd \\ Ca & Cb & Da & Db \\ Cc & Cd & Dc & Dd \end{pmatrix} \quad . \tag{5}$$

The point to be emphasized is that in (3) and (4), by reversing the order of the extended product, we succeed in distinguishing the S^+ operators of the two sites by two different (extended) matrices as if the i labels $i = 1, 2$ were built into the final matrices. Of course, the extended matrices S_i^+, S_i^- and S_i^z are true spins: they obey the commuting spin rules (e. g. $[S_i^+, S_j^-]_- = 2\delta_{i,j} S_i^z$).

The next step is to obtain an extended matrix for the Hamiltonian (see Appendix A). Finally,one constructs the chain of equations, using matrix multiplication in the evaluation of $[S_i^+, \mathcal{H}]_-$, etc. The following procedure will always be followed (see section 3): we begin calculating the commutator $[S_i^+, \mathcal{H}]_-$ as difference between product of matrices. The resulting matrix is (tentatively) decomposed as a sum of two terms: the first one being proportional to the matrix S_1^+ and a remaining term A_1. This same pattern applies to the matrix A_1 (in the place of S_1^+), etc.

We obtain

$$[S_1^+, \mathcal{H}]_- = \mu h S_1^+ + J A_1 \tag{6}$$

$$[A_1, \mathcal{H}]_- = 2J S_1^+ + \mu h A_1 - 2J A_2 \tag{7}$$

$$[A_2, \mathcal{H}]_- = -J A_1 + \mu h A_2 \quad . \tag{8}$$

The matrices A_1 and A_2 are given in Appendix A. Equations (6-8) are easily obtained using CA. From (2) and (6-8) we have

$$\begin{pmatrix} E & -J & 0 \\ -2J & E & 2J \\ 0 & J & E \end{pmatrix} \begin{pmatrix} \langle S_1^+ \mid S_1^- \rangle \\ \langle A_1 \mid S_1^- \rangle \\ \langle A_2 \mid S_1^- \rangle \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} 2\langle S_1^z \rangle \\ \langle [A_1, S_1^-]_- \rangle \\ \langle [A_2, S_1^-]_- \rangle \end{pmatrix} . \tag{9}$$

The transition energies are then given by

$$det \begin{pmatrix} E & -J & 0 \\ -2J & E & 2J \\ 0 & J & E \end{pmatrix} = 0 \qquad . \tag{10}$$

Where $E = w - \mu h$.

Equation (10) is the same as

$$E(E-2J)(E+2J) = 0 \tag{11}$$

and the poles w's are

$$w_1 = \mu h, \qquad\qquad w_{2,3} = \mu h \pm 2J \qquad . \tag{12}$$

In (9), $[A_1, S_1^-]_-$ is easily identified as $4S_1^z S_2^z + 2S_2^+ S_1^-$ and $[A_2, S_1^-]_- = 0$.

The GF $\langle S_1^+ \mid S_1^- \rangle$, obtained from (9) is

$$\begin{aligned} \langle S_1^+ \mid S_1^- \rangle \;\; &= \;\; \frac{\langle S_1^z \rangle}{\pi E} + \frac{2J^2 \langle S_1^z \rangle}{\pi E(E-2J)(E+2J)} + \frac{2J \langle S_1^z S_2^z \rangle}{\pi (E-2J)(E+2J)} + \\ &+ \frac{J \langle S_2^+ S_1^- \rangle}{\pi (E-2J)(E+2J)} \qquad . \end{aligned} \tag{13}$$

Expression (13) is the same as that of Lucas (eq.6 of ref. 6.)

Still, for the two-spin cluster, but now with $S = 1$, we have

$$[S_1^+, \mathcal{H}]_- = \mu h S_1^+ + 2JA_1 \tag{14}$$

$$[A_1, \mathcal{H}]_- = 2JS_1^+ + \mu h A_1 + 2JA_2 \tag{15}$$

$$[A_2, \mathcal{H}]_- = 2JA_1 + \mu h A_2 + 2JA_3 \tag{16}$$

$$[A_3, \mathcal{H}]_- = 2JS_1^+ + 2JA_2 + \mu h A_3 + 4JA_4 \tag{17}$$

$$[A_4, \mathcal{H}]_- = 2JA_3 + \mu h A_4 \qquad . \tag{18}$$

Of course, here the A's are not those that appear on (6-8); we maintain the some notation (now and further on) for the sake of uniformity. Also the $\mathbf{S}_1$ (S_1^+, S_1^-, S_1^z) operators are 9 x 9 matrices defined in a similar way to (3-5).

From (2) and (14-18) we get

$$\begin{pmatrix} E & -2J & 0 & 0 & 0 \\ -2J & E & -2J & 0 & 0 \\ 0 & -2J & E & -2J & 0 \\ -2J & 0 & -2J & E & -4J \\ 0 & 0 & 0 & -2J & E \end{pmatrix} \begin{pmatrix} \langle S_1^+ \mid S_1^- \rangle \\ \langle A_1 \mid S_1^- \rangle \\ \langle A_2 \mid S_1^- \rangle \\ \langle A_3 \mid S_1^- \rangle \\ \langle A_4 \mid S_1^- \rangle \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} 2\langle S_1^z \rangle \\ \langle [A_1, S_1^-]_- \rangle \\ \langle [A_2, S_1^-]_- \rangle \\ \langle [A_3, S_1^-]_- \rangle \\ \langle [A_4, S_1^-]_- \rangle \end{pmatrix} .$$

(19)

The transition energies are obtained from

$$E(E-2J)(E+2J)(E-4J)(E+4J) \quad = \quad 0 \qquad . \tag{20}$$

Again $E = w - \mu h$. From (20) we get

$$w_1 = \mu h, \qquad\qquad w_{2,3} = \mu h \pm 2J, \qquad\qquad w_{4,5} = \mu h \pm 4J \tag{21}$$

and from (19)

$$\begin{aligned}
\langle S_1^+ \mid S_1^- \rangle \quad = \quad & \frac{E\langle S_1^z\rangle}{\pi E(E-2J)(E+2J)} + \frac{32J^4\langle S_1^z\rangle}{\pi E(E-2J)(E+2J)(E-4J)(E+4J)} + \\
& \frac{J\langle [A_1, S_1^-]_-\rangle (E-2J\sqrt{3})(E+2J\sqrt{(3)})}{\pi(E-2J)(E+2J)(E-4J)(E+4J)} + \\
& \frac{2EJ^2\langle [A_2, S_1^-]_-\rangle}{\pi(E-2J)(E+2J)(E-4J)(E+4J)} + \\
& \frac{4J^3\langle [A_3, S_1^-]_-\rangle}{\pi(E-2J)(E+2J)(E-4J)(E+4J)} \qquad .
\end{aligned} \tag{22}$$

In (22) $[A_i, S_1^-]_-$ $(i = 1, 2, 3)$ are 9 x 9 matrices easily obtainable, but difficult to identify as sum of products of spin operators.

Before going to larger clusters (section 3), we must mention that we have learned about extended matrices in the book of the Poole and Farach[11]; they have used them to construct spin Hamiltonian matrices of interest to NMR and ESR.

3. Spin clusters with more than two spins

For three spins we have two possibilities: a triangular or a linear geometry. For three spins on the vertices of a triangle, we have each spin interacting with the two remaining ones,

$$\begin{aligned}
\mathcal{H} \quad = \quad & -J[(S_1^+.S_2^- + S_1^-.S_2^+ + 2S_1^z.S_2^z) + (S_2^+.S_3^- + S_2^-.S_3^+ + 2S_2^z.S_3^z) + \\
& (S_3^+.S_1^- + S_3^-.S_1^+ + 2S_3^z.S_1^z)] - \mu h(S_1^z + S_2^z + S_3^z) \qquad .
\end{aligned} \tag{23}$$

In the case of three spins on a line, the spin in the center (say $\mathbf{S}_2$) interacts with the spins $\mathbf{S}_1$ and $\mathbf{S}_3$,

$$\begin{aligned}
\mathcal{H} \quad = \quad & -J[(S_2^+.S_1^- + S_2^-.S_1^+ + 2S_2^z.S_1^z) + (S_2^+.S_3^- + S_2^-.S_3^+ + 2S_2^z.S_3^z)] - \\
& \mu h(S_1^z + S_2^z + S_3^z) \qquad .
\end{aligned} \tag{24}$$

The extended matrices representing S_1^+, S_2^+ and S_3^+ for $S=1/2$ are obtained as

$$S_1^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{25}$$

$$S_2^+ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{26}$$

$$S_3^+ = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad . \tag{27}$$

Similar expressions for the other spin components (S_i^- and S_i^z, $i=1,2,3$).

For $S=1/2$, despite the differences in the two spins configurations (and equations (23) and (24)), the following equations

$$[S_2^+, \mathcal{H}]_- = \mu h S_2^+ + J A_1 \tag{28}$$

$$[A_1, \mathcal{H}]_- = 2J S_2^+ + \mu h A_1 + J A_2 \tag{29}$$

$$[A_2, \mathcal{H}]_- = 7J A_1 + \mu h A_2 \tag{30}$$

apply to both cases. They exhibit the same energy transitions; but (see section 4.1) the triangular configuration has degeneracies in the energy levels not present in the linear arrangement, which has less symmetry. It is worth noting that the GF method works only (in the case of the three spins on a line) if we choose $\langle S_2^+ \mid S_j^- \rangle$ for the GF; if we had started with $\langle S_1^+ \mid S_j^- \rangle$ or $\langle S_3^+ \mid S_j^- \rangle$ the corresponding equations to (28-30) would have increased indefinitely. The same problem occurs with larger clusters. In order to obtain a closed system of equations one has to work with a spin sitting in a position which connects with all other sites and these have to be nearest neighbors. From (28-30) we obtain

$$\begin{pmatrix} w-\mu h & -J & 0 \\ -2J & w-\mu h & -J \\ 0 & -7J & w-\mu h \end{pmatrix} \begin{pmatrix} \langle S_2^+ \mid S_2^- \rangle \\ \langle A_1 \mid S_2^- \rangle \\ \langle A_2 \mid S_2^- \rangle \end{pmatrix} = \frac{1}{2\pi} \begin{pmatrix} 2\langle S_2^z \rangle \\ \langle [A_1, S_2^-]_- \rangle \\ \langle [A_2, S_2^-]_- \rangle \end{pmatrix} \tag{31}$$

and the transition energies are

$$w_1 = \mu h, \qquad w_{2,3} = \mu h \pm 3J \tag{32}$$

and

$$\langle S_2^+ \mid S_2^- \rangle = \frac{E\langle S_2^z \rangle}{\pi(E-3J)(E+3J)} - \frac{7J^2\langle S_2^z\rangle}{\pi E(E-3J)(E+3J)} + \frac{J\langle [A_1, S_2^-]_-\rangle}{2\pi(E-3J)(E+3J)} + \frac{J^2\langle [A_2, S_2^-]_-\rangle}{2\pi E(E-3J)(E+3J)} \tag{33}$$

where $E = w - \mu h$. The average values of the right hand side of (33) will be computed in section 4.2. Similar results for $S = 1$ are given in Appendix B.

Now we present results for clusters of four spins. There are two simple cases: three spins on the vertices of an (equilateral) triangle and a fourth spin on the geometric center of the triangle; in the other possibility the fours spins are on the vertices of a tetrahedron. The two cases have the following Hamiltonians

$$\begin{aligned} \mathcal{H} &= -J[(S_1^+.S_2^- + S_1^-.S_2^+ + 2S_1^z.S_2^z) + (S_1^+.S_3^- + S_1^-.S_3^+ + 2S_1^z.S_3^z) + \\ &\quad (S_1^+.S_4^- + S_1^-.S_4^+ + 2S_1^z.S_4^z)] - \mu h(S_1^z + S_2^z + S_3^z + S_4^z) \end{aligned} \tag{34}$$

and

$$\begin{aligned} \mathcal{H} &= -J[(S_1^+.S_2^- + S_1^-.S_2^+ + 2S_1^z.S_2^z) + (S_1^+.S_3^- + S_1^-.S_3^+ + 2S_1^z.S_3^z) + \\ &\quad (S_1^+.S_4^- + S_1^-.S_4^+ + 2S_1^z.S_4^z) + (S_2^+.S_3^- + S_2^-.S_3^+ + 2S_2^z.S_3^z) + \\ &\quad (S_2^+.S_4^- + S_2^-.S_4^+ + 2S_2^z.S_4^z) + (S_3^+.S_4^- + S_3^-.S_4^+ + 2S_3^z.S_4^z)] - \\ &\quad - \mu h(S_1^z + S_2^z + S_3^z + S_4^z) \quad . \end{aligned} \tag{35}$$

The extended representation of the four spins $\mathbf{S}_i$,$(i = 1, 2, 3, 4)$, follows the same pattern of the three spin cluster

$$S_1^+ = S^+ \otimes \Box \otimes \Box \otimes \Box \tag{36}$$

$$S_2^+ = \Box \otimes S^+ \otimes \Box \otimes \Box \tag{37}$$

$$S_3^+ = \Box \otimes \Box \otimes S^+ \otimes \Box \tag{38}$$

$$S_4^+ = \Box \otimes \Box \otimes \Box \otimes S^+ \quad . \tag{39}$$

Where S^+ is the Pauli matrix $\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $\Box$ is a 2 x 2 unit matrix. For both Hamiltonians, we have $(S = 1/2)$

$$[S_1^+, \mathcal{H}]_- = \mu h S_1^+ + JA_1 \tag{40}$$

$$[A_1, \mathcal{H}]_- = 4JS_1^+ + \mu h A_1 + 2JA_2 \tag{41}$$

$$[A_2, \mathcal{H}]_- = 6JA_1 + \mu h A_2 + 2JA_3 \tag{42}$$

$$[A_3, \mathcal{H}]_- = (\mu h + 2J)A_3 + 4JA_4 \tag{43}$$

$$[A_4, \mathcal{H}]_- = (\mu h - 2J)A_4 \tag{44}$$

Following the same steps as we did in the case of the three spins, we get

$$w_1 = \mu h, \qquad w_{2,3} = \mu h \pm 2J, \qquad w_{4,5} = \mu h \pm 4J \tag{45}$$

and

$$\langle S_1^+ \mid S_1^- \rangle = \frac{E\langle S_1^z\rangle}{\pi(E-4J)(E+4J)} - \frac{12J^2\langle S_1^z\rangle}{\pi E(E-4J)(E+4J)} + \frac{J\langle [A_1, S_1^-]_-\rangle}{2\pi(E-4J)(E+4J)} + \frac{J^2\langle [A_2, S_1^-]_-\rangle}{2\pi E(E-4J)(E+4J)} \quad . \tag{46}$$

Again, both plane and tetrahedral geometries have the same excitation energies; however, (see Section 4.1) the tetrahedral configuration has degenerate energy levels.

For five spins ($S = 1/2$) sitting on the vertices and at the center of a tetrahedron, we get the following results

$$[S_1^+, \mathcal{H}]_- = \mu h S_1^+ + JA_1 \tag{47}$$

$$[A_1, \mathcal{H}]_- = 4JS_1^+ + \mu h A_1 + JA_2 \tag{48}$$

$$[A_2, \mathcal{H}]_- = 21JA_1 + \mu h A_2 + 8JA_3 \tag{49}$$

$$[A_3, \mathcal{H}]_- = (\mu h + 3J)A_3 + JA_4 \tag{50}$$

$$[A_4, \mathcal{H}]_- = (\mu h - 3J)A_4 \tag{51}$$

and

$$\begin{aligned}\langle S_1^+ \mid S_1^- \rangle \;=\; & \frac{\langle S_1^z\rangle(E-J\sqrt{21})(E+J\sqrt{21})}{\pi E(E-5J)(E+5J)} - \frac{J\langle [A_1, S_1^-]_-\rangle}{2\pi(E-5J)(E+5J)} + \\ & \frac{J^2\langle [A_2, S_1^-]_-\rangle}{2\pi E(E-5J)(E+5J)} + \frac{8J^3\langle [A_3, S_1^-]_-\rangle}{2\pi E(E+3J)(E-5J)(E+5J)} \\ & + \frac{8J^4\langle [A_4, S_1^-]_-\rangle}{2\pi E(E-3J)(E+3J)(E-5J)(E+5J)}\end{aligned} \tag{52}$$

where $E = w - \mu h$

and

$$E(E-3J)(E+3J)(E-5J)(E+5J) = 0 \quad . \tag{53}$$

The excitation energies w's are

$$w_1 = \mu h \qquad w_{2,3} = \mu h \pm 3J \qquad w_{4,5} = \mu h \pm 5J \qquad . \tag{54}$$

In obtaining (47-51) and (52), we have assumed that the spins $\mathbf{S}_1$ is in the center of the tetrahedron and interacts with the other four spins;

$$\begin{aligned} \mathcal{H} \;=\; & -J[(S_1^+.S_2^- + S_1^-.S_2^+ + 2S_1^z.S_2^z) + (S_1^+.S_3^- + S_1^-.S_3^+ + 2S_1^z.S_3^z) + \\ & (S_1^+.S_4^- + S_1^-.S_4^+ + 2S_1^z.S_4^z) + (S_1^+.S_5^- + S_1^-.S_5^+ + 2S_1^z.S_5^z) + \\ & \mu h(S_1^z + S_2^z + S_3^z + S_4^z + S_5^z) \qquad . \end{aligned} \tag{55}$$

The extended representation of the five spins $\mathbf{S}_i$, $i = 1, 2, 3, 4, 5$, is similar to the four spins case.

Finally we consider three spins on a line, one having a different spin quantum number. The Hamiltonian is

$$\begin{aligned} \mathcal{H} \;=\; & -J[(S_2^+.s_1^- + S_2^-.s_1^+ + 2S_2^z.s_1^z) + (S_2^+.s_3^- + S_2^-.s_3^+ + 2S_2^z.s_3^z)] - \\ & \mu h(s_1^z + S_2^z + s_3^z) \qquad . \end{aligned} \tag{56}$$

The spins at sites one and three having quantum number $S = 1/2$; spin at sites two has $S = 1$. The extended spin representation now is the following

$$s_1^+ = s^+ \otimes \Box_3 \otimes \Box_2 \tag{57}$$

$$S_2^+ = \Box_2 \otimes S^+ \otimes \Box_2 \tag{58}$$

$$s_3^+ = \Box_2 \otimes \Box_3 \otimes s^+ \tag{59}$$

where $\Box_i$ $(i = 2, 3)$, refers to a unit matrix of dimension i x i.

The equations of motion are

$$[S_2^+, \mathcal{H}] = \mu h S_2^+ + 2JA_1 \tag{60}$$

$$[A_1, \mathcal{H}] = 2JS_2^+ + \mu h A_1 + JA_2 \tag{61}$$

$$[A_2, \mathcal{H}] = 12JA_1 + \mu h A_2 + 2JA_3 \tag{62}$$

$$[A_3, \mathcal{H}] = (\mu h + J)A_3 + JA_4 \tag{63}$$

$$[A_4, \mathcal{H}] = 2JA_3 + \mu h A_4 + 4JA_5 \tag{64}$$

$$[A_5, \mathcal{H}] = (\mu h - 2J)A_5 \tag{65}$$

From (60 - 65) we obtain

$$\begin{aligned}\langle S_2^+ \mid S_2^- \rangle &= \frac{\langle S_2^z\rangle(E-J\sqrt{12})(E+J\sqrt{12})}{\pi E(E-4J)(E+4J)} - \frac{J\{E\langle[A_1,S_2^-]\rangle + J\langle[A_2,S_2^-]\rangle\}}{\pi E(E-4J)(E+4J)} - \\ &\frac{2J^3\{\langle E[A_3,S_2^-]\rangle + J\langle[A_4,S_2^-]\rangle\}}{\pi E(E-J)(E+2J)(E-4J)(E+4J)} - \\ &\frac{8J^5\langle[A_5,S_2^-]\rangle}{\pi E(E-J)(E-2J)(E+2J)(E-4J)(E+4J)} \end{aligned} \quad (66)$$

and the poles w's are

$$w_1 = \mu h, \qquad w_2 = \mu h - J, \qquad w_{3,4} = \mu h \pm 2J, \qquad w_{5,6} = \mu h \pm 4J \quad . \quad (67)$$

If for the spins at the ends of the line, $S = 1$ and at the center $S = 1/2$, we have

$$S_1^+ = S^+ \otimes \Box_2 \otimes \Box_3 \quad (68)$$

$$s_2^+ = \Box_3 \otimes S^+ \otimes \Box_3 \quad (69)$$

$$S_3^+ = \Box_3 \otimes \Box_2 \otimes S^+ \quad (70)$$

where $\Box_i$ $(i = 2,3)$, refers to a unity matrix of i x i dimension.

The equations of motion are

$$[s_2^+, \mathcal{H}] = \mu h s_2^+ + J A_1 \quad (71)$$

$$[A_1, \mathcal{H}] = \mu h A_1 + 4J s_2^+ + J A_2 \quad (72)$$

$$[A_2, \mathcal{H}] = \mu h A_2 + 21 J A_1 + 8 J A_3 \quad (73)$$

$$[A_3, \mathcal{H}] = (\mu h + 3J) A_3 + 2J A_4 \quad (74)$$

$$[A_4, \mathcal{H}] = (\mu h - 3J) A_4 \quad (75)$$

$$\begin{aligned}\langle s_2^+ \mid s_2^- \rangle &= \frac{\langle s_2^z\rangle(E-J\sqrt{21})(E+J\sqrt{21})}{\pi E(E-5J)(E+5J)} + \frac{J\{E\langle[A_1,s_2^-]\rangle + J\langle[A_2,s_2^-]\rangle\}}{2\pi E(E-5J)(E+5J)} + \\ &\frac{4J^3\langle E[A_3,s_2^-]\rangle}{\pi E(E+3J)(E-5J)(E+5J)} + \\ &\frac{8J^4\langle[A_4,s_2^-]\rangle}{\pi E(E-3J)(E+3J)(E-5J)(E+5J)} \end{aligned} \quad (76)$$

and the poles w's are

$$w_1 = \mu h \qquad w_{2,3} = \mu h \pm 3J \qquad w_{4,5} = \mu h \pm 5J \quad . \quad (77)$$

The results in this section were obtained using CA to calculate the commutators $[S_2^+, \mathcal{H}]_-$, etc (e.g. 28-30) and in factorizing the denominators of the Green Functions.

4. Energy Levels and Statistical averages

In this section we make use of the extended spin representation to obtain the energy levels for most of the clusters presented in section 3. Besides being of interest by themselves, they are also needed if one wants to compute average values.

4.1 Energy levels

The energy levels are obtained from the roots y_i of the characteristic equation

$$det \mid < m \mid \mathcal{H} \mid m > -y\delta_{m,n} \mid = 0 \tag{78}$$

where $< m \mid \mathcal{H} \mid n >$ are directly read from the extended representation of the Hamiltonians.

4.1.1 Two-Spin System $S = 1/2$

$$y_1 = -\mu h - \frac{J}{2} \qquad y_2 = -\frac{J}{2} \qquad y_3 = \mu h - \frac{J}{2} \qquad y_4 = \frac{3J}{2} \tag{79}$$

This is the simplest (and trivial) case. The excitations energies (see section 2) correspond to the following energy differences

$$\begin{aligned} w_1 &= y_3 - y_2 = y_2 - y_1 = \mu h, \\ w_2 &= y_4 - y_1 = \mu h + 2J, \\ w_3 &= y_3 - y_4 = \mu h - 2J \quad . \end{aligned} \tag{80}$$

4.1.2 Two-Spin System $(S = 1)$

$$y_1 = -2\mu h - 2J \qquad y_2 = -\mu h - 2J \qquad y_3 = -\mu h + 2J \tag{81}$$

$$y_4 = -2J \qquad y_5 = \mu h - 2J \qquad y_6 = 2J \tag{82}$$

$$y_7 = 4J \qquad y_8 = \mu h + 2J \qquad y_9 = 2\mu h - 2J \tag{83}$$

4.1.3 Three Spins on a line / the vertices of a triangle

In the first case we have

$$\begin{array}{rclrclrcl} y_1 &=& -\frac{3\mu h+2J}{2} & y_2 &=& \frac{3\mu h-2J}{2} & y_3 &=& \frac{\mu h-2J}{2} \\ y_4 &=& -\frac{\mu h}{2} & y_5 &=& \frac{\mu h}{2} & y_6 &=& -\frac{\mu h+2J}{2} \\ y_7 &=& \frac{\mu h+4J}{2} & y_8 &=& -\frac{\mu h-4J}{2} & & & . \end{array} \tag{84}$$

For the spins on the vertices of a triangle

$$\begin{array}{rclrclrcl} y_1 &=& -\frac{3(\mu h+J)}{2} & y_2 &=& \frac{3(\mu h-J)}{2} & y_3 &=& -\frac{\mu h+3J}{2} \\ y_4^d &=& \frac{\mu h+3J}{2} & y_5 &=& \frac{\mu h+3J}{2} & y_6^d &=& -\frac{\mu h-3J}{2} \end{array} \tag{85}$$

we note that in the last case there are energy degeneracies (the superscript d refers to doublet); otherwise the energy levels are the some as for the more symmetrical geometry (three spin on the vertices of the triangle).

4.1.4 Four Spins Cluster

For four spins (three on the vertices and one at the center of an equilateral triangle) we have

$$\begin{array}{rclrclrcl} y_1 &=& -2\mu h-\frac{3J}{2} & y_2 &=& -\mu h-\frac{3J}{2} & y_3^d &=& -\mu h-\frac{J}{2} \\ y_4 &=& -\mu h+\frac{5J}{2} & y_5 &=& -\frac{3J}{2} & y_6^d &=& -\frac{J}{2} \\ y_7^d &=& \frac{3J}{2} & y_8 &=& \frac{5J}{2} & y_9 &=& \mu h-\frac{3J}{2} \\ y_{10}^d &=& \mu h-\frac{J}{2} & y_{11} &=& \mu h+\frac{5J}{2} & y_{12} &=& 2\mu h-\frac{3J}{2} \quad . \end{array} \tag{86}$$

If the four spins are on the vertices of tetrahedron

$$\begin{array}{rclrclrcl} y_1 &=& -2\mu h-3J & y_2 &=& -\mu h-3J & y_3^t &=& -\mu h-J \\ y_4 &=& -3J & y_5^t &=& J & y_6 &=& \mu h-3J \\ y_7^d &=& 3J & y_8^t &=& \mu h+J & y_9 &=& 2\mu h+3J \quad . \end{array} \tag{87}$$

Again here we have degeneracies (the superscripts d and t refer to doublet and triplet, respectively).

Finally, we present results for a mixed case: on a line we have two spins ($S = 1/2$) and a spin $S = 1$, in the center.

The results are

$$\begin{aligned} y_1 = -2(J+\mu h) \qquad y_2 = -2J-\mu h \qquad y_3 &= -2J+\mu h \\ y_4 = -2(J-\mu h) \qquad y_5 = -2J \qquad y_6 &= -\mu h \\ y_7 = 0 \qquad y_8 = \mu h \qquad y_9 &= 2J-\mu h \\ y_{10} = 2J \qquad y_{11} = 2J+\mu h \qquad y_{12} &= 4J \quad . \end{aligned} \tag{88}$$

For the reversed situation: a spin $S = 1/2$ in the center and two spins $S = 1$ on the ends, we have

$$\begin{array}{lll} y_1 = -2J - \frac{5\mu h}{2} & y_2 = -2J - \frac{3\mu h}{2} & y_3 = -2J - \frac{\mu h}{2} \\ y_4 = -2J + \frac{\mu h}{2} & y_5 = -2J + \frac{3\mu h}{2} & y_6 = -2J + \frac{5\mu h}{2} \\ y_7 = -J - \frac{3\mu h}{2} & y_8 = -J - \frac{\mu h}{2} & y_9 = -J + \frac{\mu h}{2} \\ y_{10} = -J + \frac{3\mu h}{2} & y_{11} = -\mu h & y_{12} = \mu h \\ y_{13} = 2J - \frac{\mu h}{2} & y_{14} = 2J + \frac{\mu h}{2} & y_{15} = 3J - \frac{3\mu h}{2} \\ y_{16} = 3J - \frac{\mu h}{2} & y_{17} = 3J + \frac{\mu h}{2} & y_{18} = 3J + \frac{3\mu h}{2} \quad . \end{array} \tag{89}$$

4.2 Average values

To illustrate how statistical averages can be obtained, we show how the mean values which appear in the GF expressions of the three spin cluster (linear geometry) can be computed.

In order to find the unitary transformation which diagonalize $\mathcal{H}$, we make use (for each y_j) of seven (of the eight) equations

$$\sum_i C_{i,j}[< i \mid \mathcal{H} \mid j > -y_j \delta_{i,j}] \ = \ 0 \tag{90}$$

and of the normalizing condition

$$\sum_i \mid C_{i,j} \mid^2 \ = \ 1 \quad . \tag{91}$$

The C matrix, given by $C_{i,j}$, is

$$C = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & -\frac{2}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & -\frac{2}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}. \quad (92)$$

We note that C is unitary. The diagonalized Hamiltonian $\bar{\mathcal{H}}$ is

$$\bar{\mathcal{H}} = C^{-1}\mathcal{H}C = \begin{pmatrix} \frac{\mu h}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\mu h}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\mu h+4J}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mu h-4J}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{3\mu h-2J}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\mu h-2J}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\mu h+2J}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3\mu h+2J}{2} \end{pmatrix} \quad (93)$$

To compute $< A >$, we first obtain $\bar{A} = C^{-1}AC$; then

$$\langle A\rangle = \langle \bar{A}\rangle = \frac{\sum_{i=1} e^{-\beta y_i}\langle i \mid \bar{A} \mid i\rangle}{\sum_{i=1} e^{-\beta y_i}} \quad (94)$$

where $\beta = \frac{1}{k_B T}$ (k_B is the Boltzmann constant and T the temperature).

The averages values which appear in the GF expression (for three spins on line) are

$$\langle S_2^z\rangle = (\frac{1}{6})\frac{sinh(\frac{\beta\mu h}{2})[1+3e^{-\beta\mu J} - e^{-3\beta\mu J}] + 3sinh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[1+e^{-\beta\mu J} + e^{-3\beta\mu J}] + cosh(\frac{3\beta\mu h}{2})} \quad (95)$$

$$\langle(\mathbf{S}_2.\mathbf{S}_1 + \mathbf{S}_2.\mathbf{S}_3)\rangle = (\frac{1}{2})\frac{cosh(\frac{\beta\mu h}{2})[1-2e^{-3\beta\mu J}] + cosh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[1+e^{-\beta\mu J} + e^{-3\beta\mu J}] + cosh(\frac{3\beta\mu h}{2})} \quad (96)$$

$$\langle[A_1, S_2^-]\rangle = (\frac{2}{3})\frac{cosh(\frac{\beta\mu h}{2})[1+4e^{-3\beta\mu J}] + 3cosh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[1+e^{-\beta\mu J} + e^{-3\beta\mu J}] + cosh(\frac{3\beta\mu h}{2})} \quad (97)$$

$$\langle [A_2, S_2^-] \rangle = (\frac{2}{3}) \frac{sinh(\frac{\beta\mu h}{2})[1 - 3e^{-\beta\mu J} - 5e^{-3\beta\mu J}] + 6sinh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[1 + e^{-\beta\mu J} + e^{-3\beta\mu J}] + cosh(\frac{3\beta\mu h}{2})} \quad (98)$$

$$\langle S_1^z \rangle = (\frac{1}{6}) \frac{sinh(\frac{\beta\mu h}{2})[1 + 2e^{-3\beta\mu J}] + 3sinh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[1 + e^{-\beta\mu J} + e^{-3\beta\mu J}] + cosh(\frac{3\beta\mu h}{2})} \quad (99)$$

$$\langle S_1^z \rangle = \langle S_3^z \rangle \neq \langle S_2^z \rangle \quad . \quad (100)$$

Results for three spins on the vertices of a triangle are given in Appendix C.

The results in this section were obtained using CA: first to factorize the characteristic polynomials (eq. 78); also to dealt with (interactively) the equations 88 and 89 to obtain the matrix C, and obtaining (93-98).

5. Summary

In retrospect, we have shown that by expanding the Hilbert space of the spin operators to accomodate the site attributes, the task of computing $[S_i^+, \mathcal{H}]_-$ is reduced to matrix algebra operations.However, the size of the extended matrices increase with the size of the cluster:e.g. the spin operators for a cluster of five spins (S=1/2) are represented by 32 x 32 matrices, although most of the their elements are zero.To handle such matrices we can use CA systems, now available in different sizes and prices, from the humble PC[12] to the powerful Workstations[13]. We have worked with a (far from today‘s top line) Reduce 2.3 version in a Sun SPARCstation 2. In this way we could derive the GF chained equations of motion for various spin clusters and solve for the GF of interest. The poles of the GF give the transition energies directly, with no need of worrying about selection rules. CA was also employed in obtaining the energy levels.

Comparing the results for different clusters we note that the GF have simple poles, except for the case of three spins, for $S = 1$, where we have a double pole. A remarkable result is that for clusters of equal number of spins, but with differents geometries, the poles of the GF are the same; however, the more symmetrical cluster has degeneracies in the energy levels, not present in the other case. It is also interesting to note that the case of three spins with different quantum numbers ($S = 1/2$) at the center and $S = 1$ at the ends) has the same transition energies of the case of five spins $S = 1/2$. For $S = 1/2$, the values of the transition energies increase with the number of spins in the cluster (note that the w's go with nJ ($n = 2, 3, 4, 5$)); the values of the energy levels also increase with the size of the cluster.

The computation of mean values, despite the fact that the dimension of the extended representation increases with the size of the cluster (2^n, for $S = 1/2$; n being the number of spins in the cluster), also proved to be particularly simple to be done via CA. Finally, it seems worth to mention that the only limiting factors, if one wants to go on for still larger clusters, are the memory and velocity of your computer; hopefully, CA combined with the proper algorithms may prompt a revival of the GF method.

Acknowledgements

We are indebted to Dr. A. P. Guimarães for helpful discussions and for reviewing the manuscript. One of the authors (RRS), acknowledges a CNPq/Brazil post-doctoral fellowship.

Appendix A

For two spins ($S = 1/2$), the Hamiltonian (1) in the extended matrix representation is

$$\mathcal{H} \;=\; \frac{1}{2}\begin{pmatrix} -2\mu h - J & 0 & 0 & 0 \\ 0 & J & -2J & 0 \\ 0 & -2J & J & 0 \\ 0 & 0 & 0 & 2\mu h - J \end{pmatrix}.$$

The left hand side commutators (6-8) are

$$[S_1^+, \mathcal{H}] = \mu h \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + J \begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \mu h S_1^+ + J A_1 \qquad (101)$$

$$[A_1, \mathcal{H}] \;=\; \mu h \begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} + 2J \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} - 2J \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} =$$

$$\mu h A_1 + 2J S_1^+ - 2J A_2 \qquad (102)$$

$$[A_2, \mathcal{H}] \;=\; \mu h \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} - J \begin{pmatrix} 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \mu h A_2 - J A_1$$

Appendix B

For two spins ($S = 1$), we have

$$[S_2^+, \mathcal{H}] = \mu h S_2^+ + 2JA_1 \tag{103}$$

$$[A_1, \mathcal{H}] = \mu h A_1 + 2JS_2^+ + 2JA_2 \tag{104}$$

$$[A_2, \mathcal{H}] = \mu h A_2 + 8JA_1 + 2JA_3 \tag{105}$$

$$[A_3, \mathcal{H}] = \mu h A_3 + 2JA_2 + 2JA_4 \tag{106}$$

$$[A_4, \mathcal{H}] = \mu h A_4 + 14JA_3 + 8JA_5 \tag{107}$$

$$[A_5, \mathcal{H}] = (\mu h - 2J)A_5 + 2JA_6 \tag{108}$$

$$[A_6, \mathcal{H}] = \mu h A_6 + 4JA_5 + 4JA_7 \tag{109}$$

$$[A_7, \mathcal{H}] = (\mu h - 2J)A_7 \tag{110}$$

$$\begin{aligned}\langle S_1^+ \mid S_1^- \rangle \;=\; & \frac{1}{2\pi(E(E-4J)(E+4J)(E+6J)(E-6J)}\{2\langle S_1^z\rangle(E+2J\sqrt{6-2\sqrt{2}}) \\ & (E-2J\sqrt{6-2\sqrt{2}})(E+2J\sqrt{6+2\sqrt{2}})(E-2J\sqrt{6+2\sqrt{2}}) + \\ & 2JE\langle[A_1, S_1^-]_-\rangle(E+4J\sqrt{2})(E-4J\sqrt{2}) + \\ & 4J^2\langle[A_2, S_1^-]_-\rangle(E+2J\sqrt{7})(E-2J\sqrt{7}) + 8J^3E\langle[A_3, S_1^-]_-\rangle + \\ & 16J^4\langle[A_4, S_1^-]_-\rangle\} + \\ & \frac{1}{2\pi E(E-2J)(E+2J)(E-4J)(E+4J)^2(E+6J)(E-6J)} \\ & \{128J^5E(E+2J)\langle[A_5, S_1^-]_-\rangle + 256J^6E\langle[A_6, S_1^-]_-\rangle + \\ & 1024J^7\langle[A_7, S_1^-]_-\rangle\}\end{aligned} \tag{111}$$

$$w_1 = \mu h \qquad w_{2,3} = \mu h \pm 2J \qquad w_{4,5} = \mu h \pm 4J \tag{112}$$

$$w_{6,7} = \mu h \pm 6J \qquad \mu h + 4J \tag{113}$$

Appendix C

Mean values for three spins (= 1/2) on the vertices of a triangle. The unitary matrix C is the same of that given in (90). The diagonalized Hamiltonian is

$$C^{-1}\mathcal{H}C = \begin{pmatrix} \frac{\mu h+3J}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\mu h-3J}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{\mu h+3J}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\mu h-3J}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3\frac{\mu h-J}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\mu h-3J}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\mu h+3J}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3\frac{3\mu h+J}{2} \end{pmatrix}. \tag{114}$$

The mean values that occur in the GF are

$$\langle S_1^z \rangle = (\frac{3}{2})\frac{sinh(\frac{\beta\mu h}{2})[2+e^{3\beta\mu J}]+3e^{3\beta\mu J}sinh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[2+e^{3\beta\mu J}]+e^{3\beta\mu J}cosh(\frac{3\beta\mu h}{2})} \tag{115}$$

$$\begin{aligned} &\langle (S_1.S_2+S_1.S_3+S_2.S_3)\rangle = \\ &(\frac{3}{4})\frac{cosh(\frac{\beta\mu h}{2})[e^{3\beta\mu J}-2]+e^{3\beta\mu J}cosh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[2+e^{3\beta\mu J}]+e^{3\beta\mu J}cosh(\frac{3\beta\mu h}{2})} \end{aligned} \tag{116}$$

$$\langle [A_1, S_1^-]\rangle = (\frac{2}{3})\frac{cosh(\frac{\beta\mu h}{2})[e^{3\beta\mu J}-4]+3e^{3\beta\mu J}cosh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[2+e^{3\beta\mu J}]+e^{3\beta\mu J}cosh(\frac{3\beta\mu h}{2})} \tag{117}$$

$$\langle [A_2, S_2^-]\rangle = (\frac{4}{3})\frac{sinh(\frac{\beta\mu h}{2})[e^{3\beta\mu J}-4]+3e^{3\beta\mu J}sinh(\frac{3\beta\mu h}{2})}{cosh(\frac{\beta\mu h}{2})[2+e^{3\beta\mu J}]+e^{3\beta\mu J}cosh(\frac{3\beta\mu h}{2})} \tag{118}$$

$$\langle S_1^z\rangle = \langle S_2^z\rangle = \langle S_3^z\rangle \tag{119}$$

$$\langle [A_1, S_1^-]\rangle = \langle [A_1, S_2^-]\rangle = \langle [A_1, S_3^-]\rangle \tag{120}$$

$$\langle [A_2, S_1^-]\rangle = \langle [A_2, S_2^-]\rangle = \langle [A_2, S_3^-]\rangle \tag{121}$$

References

[1] N. N. Bogolyubov and S. V. Tyablikov, "Retarded and advanced Green Functions in statistical physics," Sov. Phys. Dokl. **4**,589-593 (1959).

[2] H. B. Callen,"Green Function Theory of Ferromagnetism," Phys. Rev. **130**, 890-898 (1963).

[3] J. Hubbard,"Electron correlation in narrow energy bands," Proc. Roy. Soc. (London) **A (276)** , 238- (1963).

[4] S. Doniach and E. H. Sondeheimer, Green Functions for Solid State Physicists, (Benjamin/Cummings, 1974).

[5] V. Yu. Irkhin and Yu. P. Irkhin,"Many-Electron Operator Approach in the the Solid State Theory," Phys. Stat. Sol. (b), **183**, 9-55 (1994).

[6] J.S. Smart, Effective Field Theories of Magnetism, (W.B. Saunders,1966).

[7] J. D. Patterson and W. H. Southwell,"Green‘s Function Theory of Ferromagnetism," Am. J. Phys. **36**, 343-350 (1968).

[8] G. L. Lucas,"Green Function Theory of the Two-Spin System," Am. J. Phys. **36** ,942-943 (1968).

[9] J. G. Ramos and A. A. Gomes,"Remarks on the Retarded, Advanced and Thermodynamic Green‘s Functions," Il Nuovo Cimento **3A**, 441-455 (1971).

[10] D. N. Zubarev, Sov. Phys. Uspekhi, **3**, 320-345 (1960)

[11] C. P. Poole and H. A. Farach, in: The Theory of Magnetic Resonance (Wiley-Interscience, 1972).

[12] W. Hereman,"Visual data analysis: maths made easy," Physics World 49-53 April 1995.

[13] J. Fitch,"Mathematics goes automatic," 48-52 Physics World June 1993.